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Application of probability circles analysis to the construction of calibration curves for infra red spectroscopy

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Abstract

A new method, based on the presentation of initial data in the form of probability circles (PC), has been developed for constructing a calibration curve, which shows a monotonic dependence with respect to the given concentration. The centre of the reference probability circle is defined by its mean value and the radius of the circle is calculated as the value of the standard deviation of the sampling considered. The comparative probability circle is defined by the same corresponding parameters but rotated, relative to the initial reference circle, by an angle, which is related to the Pearson's correlation coefficient (PCC). The two parameters of the PCC and the statistical proximity factor (PCF), which defines the positions of the centres of the circles relative to each other, can be chosen as statistical parameters for the construction of the desired calibration curve. Experiments realized with the mixture of two liquids (chloroform serves as the basic matrix) and acetone (serves as an additive) confirm the efficiency of this new analytical method and demonstrate a possible increase sensitivity for the detection of lower concentration limit by approximately one order of magnitude. This new approach, which is free from model assumptions, and having very clear geometrical meaning, can be applied for different types of spectra and has many potential applications in the construction of calibration curves for different additives embedded within different matrices.

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1. Introduction and formulation of the problem

The detection of small concentrations of one substance within a matrix of another substance (e.g., dilute solutes in solution) presents itself as a usual task for analytical science. Current procedures often involve sample concentration, derivitization and/or the separation of the mixture into component parts (e.g., chromatography); followed by measurement using some chemical or physical technique (such as chemical titration or spectroscopy). Invariably these procedures are time consuming and expensive, and require considerable investment in equipment, time and skilled staff. In many cases the manipulation of the sample (e.g., by concentration) is not an option and so the issue turns to a question of the sensitivity and selectivity of existing measurement techniques. Levels of detection can be improved by attempts to increase the signal to noise ratio, but this adds to the cost of instrumentation. An alternative and potentially more cost-effective option would be to develop new methodologies to improve the recognition and quantification of signals within otherwise random data.

A number of signal-processing methods have been developed in order to solve this problem, for example, Hurst analysis of fractal random samplings [1], wavelet-analysis, [2–5], and the stochastic dynamics of time correlations with discrete current time [6]. However, these current methods are, in part, dependent on the statistical characteristics of the

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